Dec. 13, 2010 **Final Exam Solutions** **Physics 347**

Your Name: _____ Your ID#:_____

The Final will run for 180 min.

There are 14 problems with a total of 114 points

Do your work on the pages of the exam.

Please make clear how you arrive at your answers. I cannot give credit for a correct answer unless I can see how you got it. I will give partial credit for answers which are partly correct.

No books or notes of any kind are allowed. A calculator is allowed with nothing stored in memory; but, there is nothing you will need it for, anyway.

A two-page formula sheet is attached at the end of your exam. Tear it off, if you find that convenient.

Page 1 (12+6)		Page 6 (10)	
Page 2 (10+4)		Page 7 (10)	
Page 3 (8)		Page 8 (8)	
Page 4 (8+8)		Pare 9 (10)	
Page 5 (6+6)		Page 10 (8)	

TOTAL (114)

Problem 1: (12 pts)
Give approximate or typical numerical values for the following:

(a) The number of moles per litre of water.

MW=16+2=18.
1 litre of water has a mass of 1000 g.
So, the number of litres is $\frac{1000}{18} = 55.5$

(b) Roughly how many carbon atoms does an E. coli cell contain?

10^{10}

(c) The Reynolds number for a cellular environment.

10^{-6}

(d) When you stretch a rubber band, does it heat or cool? Why?

It heats. Rubber is an entropic material, like a polymer but unlike a spring. It has no way of storing elastic energy. When you stretch it, the number of configurations decreases; therefore, the entropy decreases. This means that there is a net flow of heat out of the material.

(e) What is the thickness of a typical biological membrane, e.g., the plasma membrane?

4 nm

(f) Here is the full Navier-Stokes equation: $\rho\frac{\partial\vec{v}}{\partial t} + \rho\left(\vec{v}\cdot\vec{\nabla}\right)\vec{v} = -\vec{\nabla}P + \eta\nabla^2\vec{v}$
Circle the term that can often be neglected when the Reynolds number is small.

Problem 2: (6 pts)
Two micron-sized spheres of the same material fall under gravity in water. One has a radius of 1 μm; the other has a radius of 2 μm:

(a) Which one falls faster? Why? (show logic)

The larger one falls faster: Newton's law reads $m\frac{dv}{dt} = -\gamma v - mg$. After a short initial transient the particles reach a downwards drift velocity of magnitude $v_d = \frac{mg}{\gamma} = \frac{\frac{4}{3}\pi R^3\left(\rho - \rho_{water}\right)g}{6\pi\eta R} \sim \frac{R^3}{R} = R^2$. Thus, the net gravitational force goes as R^3 while the net drag goes only as R.
Note that the buoyant force due to the water displaced does not change this result.

(b) By what factor?

4x

Problem 3: (10 points)

Human DNA:

(a) What is the length of the human genome in meters?

$$\left(3\times10^{9}\ bp\right)\cdot\left(1/3\ nm/bp\right)=10^{9}\ nm=\boxed{1\ m}$$

(b) What is the radius of the minimum spherical volume into which it can be packed?

$$\left(3\times10^{9}\ bp\right)\cdot\left(\ nm^{3}/bp\right)=3\times10^{9}\ nm^{3}=\frac{4\pi}{3}R^{3}\ \Rightarrow\ \boxed{R=89\ nm}$$

(c) Suppose this DNA were in a single long polymer (rather than broken up into separate chromosomes). What would be the RMS end-to-end length if it were in a random-coil state? (the persistence length of DNA is $\xi_{DNA}=53\,\text{nm}$)

$$\left\langle R^{2}\right\rangle=\ell_{K}L=2\xi_{p}L=2(53)\left(10^{9}\right)\ \Rightarrow\ \sqrt{\left\langle R^{2}\right\rangle}=3.3\times10^{5}\ nm=\boxed{0.33\ mm}$$

Problem 4: (4 points)

A monomer A can form dimers and trimers according to

$A+A\leftrightarrow A_2$ and

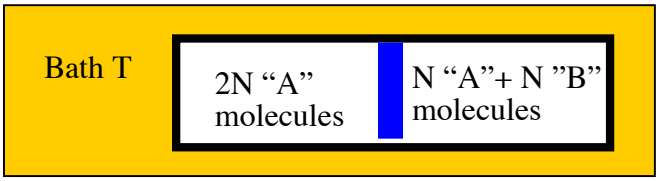
$A+A+A\leftrightarrow A_3$.

At equilibrium, what is the relation between the chemical potentials of the species A_2 and A_3?

According to the rules: $\begin{matrix}2\mu_A=\mu_{A_2}\\ 3\mu_A=\mu_{A_3}\end{matrix}$. Hence, $\boxed{\mu_{A_3}=\frac{3}{2}\mu_{A_2}}$.

Problem 5 (8 pts)

The picture at the right shows a container divided in half by a piston which is initially fixed and impermeable. The container is in a thermal bath at temperature T.



The left hand side contains 2N molecules of an ideal gas A. The right side contains N molecules of A plus another N molecules of a different gas B.

At time t=0 the piston is made semipermeable, so A's can pass through freely but B's cannot.

After the system has re-equilibrated:

(a) (My earlier version had a typo here)

The number of A molecules on the left is: (circle one) less than/ equal to/ greater than/ the number on the right. since molecules have moved from left to right

(b)

The pressure on the left is: (circle one) less than/ equal to/ greater than/ the pressure on the right. since molecules have moved from left to right and P~N

(c)

The chemical potential of A molecules on the left is: (circle one)) less than/ equal to/ greater than/ the chemical potential of A molecules on the right. that's the condition for equilibrium

(d)

The total energy of the particles in the whole container (both halves) is now:

(circle one) less than/ equal to/ greater than/ what it was at t=0.

temperature is the same, so all molecules have the same average energy ($\frac{3}{2}k_BT$ for monatomic gas).

(e)

The total entropy of the particles in the whole container is now:

(circle one) less than/ equal to/ greater than/ what it was at t=0.

The A molecules now have more volume available to them, so their entropy increases.

After this new equilibrium has been established, the piston is now allowed to move freely, while remaining semi-permeable. After the piston comes to rest:

(f)

Its final position is (circle one)

all the way to the left/ part way to the left / unchanged/ part way to the right/ all the way to the right

The total density of molecules (which determines the pressure) is always larger at the right, because of the B molecules which cannot go to the left.

(g)

The total energy of the particles in the whole container is now:

(circle one) less than/ equal to/ greater than/ what it was before the piston was made free to move.

Same logic as in (d).

(h)

The total entropy of the particles in the two containers is now:

(circle one) less than/ equal to/ greater than/ what it was before the piston was made free to move.

In this process the B molecules have access to larger volume, so it is their entropy which has increased.

Problem 6: (8 points)
You toss a coin N times (N even).
(a) What is the probability that it comes up heads *exactly* N/2 times?
(Do NOT assume here that N is large.)

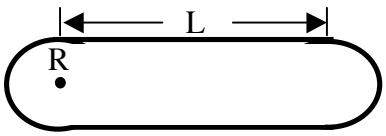
The probability of each microstate is $\frac{1}{2^N}$. The number of microstates which give exactly N/2 heads is the number of ways of choosing N/2 objects from N, so $P = \boxed{\frac{1}{2^N}\frac{N!}{\left(\frac{N}{2}!\right)^2}}$.

(b) Suppose now that N>>1. Show that this probability becomes $\sqrt{\frac{2}{\pi N}}$.

Use the Stirling formula:

$$P = \frac{1}{2^N}\cdot\frac{N!}{\left(\frac{N}{2}!\right)^2} = \frac{1}{2^N}\cdot\frac{\sqrt{2\pi N}\,N^N e^{-N}}{\left(\sqrt{\pi N}\left(\frac{N}{2}\right)^{N/2}e^{-N/2}\right)^2} = \frac{1}{2^N}\cdot\frac{\sqrt{2\pi N}}{\pi N}\cdot\left(\frac{N}{N/2}\right)^N = \boxed{\sqrt{\frac{2}{\pi N}}}.$$

Problem 7: (8 points)
A cell membrane has the shape of a cylinder of length L closed at each end by hemispherical caps of radius R. Assuming that the membrane material has no spontaneous curvature (i.e., that it is flat in its relaxed configuration), calculate the bending energy of the membrane in terms of κ_b and the cellular dimensions.



For the caps, the total area is $4\pi R^2$ and the two principal radii of curvature are both R, so

$$E_{caps} = \frac{\kappa_b}{2}\left(4\pi R^2\right)\left(\frac{1}{R}+\frac{1}{R}\right)^2 = 8\pi\kappa_b.$$

For the cylindrical region, the total area is $2\pi RL$ and the principal radii of curvature are R and ∞. so

$$E_{cylinder} = \frac{\kappa_b}{2}(2\pi RL)\left(\frac{1}{R}+\frac{1}{\infty}\right)^2 = \pi\kappa_b\frac{L}{R}.$$

Thus, the total is $\boxed{E_{total} = \pi\kappa_b\left(8+\frac{L}{R}\right)}$.

Problem 8: (6 points)

The drag force on a spherical particle of radius R moving at speed v through a viscous fluid is at low speed (low Reynolds number) is $F_{drag} = 6\pi\eta Rv$ (Stokes Law). At higher speeds the drag force increases and crosses over to a dependence on v^2 at high speed.

In the high-speed regime, what is the dependence of the drag force on the dimensional parameters R,ρ,η, i.e., $F_{drag} = C\rho^x\eta^y R^z v^2$ with what powers x,y, and z? (C is a dimensionless constant.)

This is just dimensional analysis:

$$[\rho] = \left[\frac{M}{L^3}\right]; [v] = \left[\frac{L}{T}\right]; [R] = [L]; [\eta] = \left[\frac{FT}{L^2}\right] = \left[\frac{M}{LT}\right]$$

But, the dimensions of $\left[\frac{F_{drag}}{v^2}\right] = \left[\frac{ML}{T^2}\cdot\frac{T^2}{L^2}\right] = \left[\frac{M}{L}\right] = \left[\rho R^2\right]$.

It follows that $F_{drag} = C\rho R^2 v^2$, i.e., x=1, y=0, and z=2.

It is interesting that the viscosity drops out!

Problem 9: (6 pts)

A certain protein molecule—approximately spherical—is placed in water solution. In solution, it releases positively charged counterions, thus developing a net negative charge -Q.

(a) Suppose there is no salt in the solution, will the released counterions form a charge cloud around the (negatively charged) protein? If so, what will the charge of that cloud be?

All the counterions go off to infinity. No charge cloud.

(b) Suppose now that there is salt in the solution (say, $Na^+ + Cl^-$). Will there be a cloud of net positive charge around the (negatively charged) protein? If so, what will the charge of that cloud be?

In this case, there is a charge cloud or net charge +Q, which entirely screens the negatively charged protein, when observed from a long distance.

This material was discussed in Tutorials 10 and 12.

A characteristic motion for E. coli is "run-and-tumble," which means that it swims ("runs") at constant speed v for a time t_1 and then, at the end of the interval, it stops and goes off randomly in a new direction for a time t_2, and so forth.

Make the following assumptions:

The "runs" are straight lines.

The "tumbles" are instantaneous.

The speed during a run is v=20 μm/s

The mean time of a run is 1 sec.

The run times are distributed randomly according to the exponential distribution $P(t) = \frac{1}{\tau} e^{-t/\tau}$.

(a) On the average, what is the mean square displacement $\langle R^2 \rangle$ of the bacterium from its starting point after a time T ? (Assume T>>1 s).

This is a random walk with variable step length.

By writing $\vec{R} = \vec{a}_1 + \vec{a}_2 + \vec{a}_3 + ...$ and

$\langle R^2 \rangle = \langle (\vec{a}_1 + \vec{a}_2 + \vec{a}_3 + ...) \cdot (\vec{a}_1 + \vec{a}_2 + \vec{a}_3 + ...) \rangle = a_1^2 + a_2^2 + a_3^2 + ... = N \langle a^2 \rangle$.

Now, each step has a length vt, so $\langle a^2 \rangle = v^2 \langle t^2 \rangle$, where $\langle t^2 \rangle$ is the mean squared run time.

Thus, $\langle t^2 \rangle = \int_0^\infty dt\, t^2 P(t) = \frac{1}{\tau} \int_0^\infty dt\, t^2 e^{-t/\tau} = \frac{\tau^3}{\tau} \int_0^\infty dx\, x^2 e^{-x} = 2\tau^2$.

It follows that $\langle a^2 \rangle = 2v^2\tau^2$.

Note that we are told that the mean run time $\langle t \rangle = \int_0^\infty dt\, tP(t) = \frac{1}{\tau} \int_0^\infty dt\, te^{-t/\tau} = \tau = 1\, s$.

After N runs, the mean total time is $T = N\langle t \rangle = N\tau$.

So, finally, $\langle R^2 \rangle = N \langle a^2 \rangle = \frac{T}{\tau} \cdot 2v^2\tau^2 = \boxed{2v^2\tau T}$.

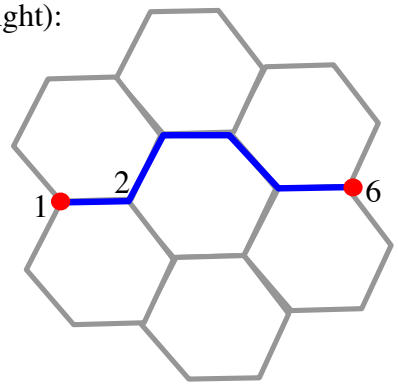
(b) What is the diffusion constant for this motion?

$\langle R^2 \rangle \sim T$, so the motion is diffusive!

This is in 3D, so $\langle R^2 \rangle = 6DT$. Comparing with (a), we find $\boxed{D = \frac{v^2\tau}{3}}$.

Problem 11 (10 points)

HP Protein folding on a honeycomb lattice (a small piece is shown at the right):
Consider an HP hexamer with the structure HPPPPH.
Each HH nearest-neighbor contact produces an energy $-\Delta$.
There are no other energies.
No two residues can occupy the same site.

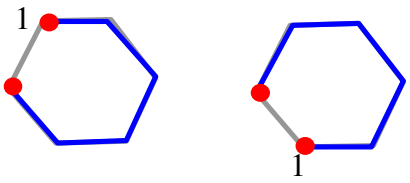


(a) How many microstates are there? (assume segment 1-2 fixed)

There are four further segments.
Each can be laid down in two possible ways.
Thus, there are $2^4 = 16$ microstates.

(b) Is there a unique native state? Explain briefly.

Yes, up to a reflection. The only way to get a nearest-neighbor HH bond is to make all four turns in the same sense, thus closing into a hexagon with the HH bond on the missing edge:



(c) What is the probability of finding this protein in its ground state at temperature T?

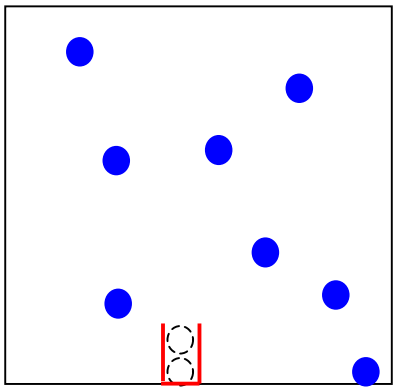
Weight all microstates with the usual canonical weighting $e^{-\beta E_n}$, so $P_{native} = \dfrac{2e^{\beta\Delta}}{14 + 2e^{\beta\Delta}}$.

Problem 12 (8 points)

Inside a volume V is an ideal gas of N molecules. On the wall of this container is a receptor site which can bind one molecule with a binding energy $-\varepsilon_B$ or two with a combined binding energy of $-(2\varepsilon_B + \Delta)$, i.e., the receptor has three states, empty, one bound ligand, and two bound ligands.

What is the probability that the site remains empty?

Hint: Use the Grand Canonical approach.



The receptor site is a small system in contact with a particle and thermal bath, thus its states are have relative weights $e^{-\beta(E_n-\mu N_n)}$. The probability that the site be empty is

$$P_{empty} = \frac{1}{1+e^{-\beta(-\varepsilon_B-\mu)}+e^{-\beta(-2\varepsilon_B-\Delta-2\mu)}} = \frac{1}{1+e^{\beta(\varepsilon_B+\mu)}+e^{\beta(2\varepsilon_B+\Delta+2\mu)}}.$$

To evaluate this, one needs the chemical potential of the ideal-gas bath.

This can be taken directly from the formula sheet: $n = \frac{N}{V} = \frac{e^{\frac{\mu}{k_B T}}}{\lambda_{th}^3} \Rightarrow \mu = k_B T \ln\left(\frac{N\lambda_{th}^3}{V}\right).$

In a two-state system, the ground state has energy $E_0 = 0$ and the excited state has energy $E_1 = \Delta$. When the system is in its excited state there is a probability per unit time k_- that it will decay to the ground state; when it is in its ground state, there is a probability per unit time k_+ that it will be thermally excited to the excited state.

(a) What is the probability at equilibrium that the system will be found in its excited state?

This is just the canonical weighting $P_1 = \dfrac{e^{-\beta E_1}}{Z} = \boxed{\dfrac{e^{-\beta\Delta}}{1+e^{-\beta\Delta}} = \dfrac{1}{e^{\beta\Delta}+1}}$.

(b) What is the relation between the rate constants k_+ and k_- required by (a)?

The rate equations are $\begin{aligned} \dfrac{dP_0}{dt} &= -k_+P_0 + k_-P_1 \\ \dfrac{dP_1}{dt} &= -k_-P_1 + k_+P_0 \end{aligned}$. Note that $\dfrac{d}{dt}\left(P_0 + P_1\right) = 0$.

At equlibrium, the time derivatives vanishe, so $k_+P_0 = k_-P_1 \quad \Rightarrow \quad \dfrac{P_1}{P_0} = \dfrac{k_+}{k_-}$.

But, from (a) $\dfrac{P_1}{P_0} = e^{-\beta\Delta}$. We conclude, $\boxed{\dfrac{P_1}{P_0} = e^{-\beta\Delta} = \dfrac{k_+}{k_-} \text{ or } \dfrac{k_-}{k_+} = e^{\beta\Delta}}$.

(c) If the system is initially in its excited state, what is the probability P(t) of finding it there at a later time t?

Using the rate equation from (b), we find $\dfrac{dP_1}{dt} = -k_-P_1 + k_+\left(1 - P_1\right) = -\left(k_- + k_+\right)P_1 + k_+$.

The general solution is $P_1(t) = \dfrac{k_+}{k_+ + k_-} + Ce^{-\left(k_+ + k_-\right)t}$.

The initial condition is $P_1(t=0) = 1$, so the solution is

$$\boxed{P_1(t) = \frac{k_+}{k_+ + k_-} + \frac{k_-}{k_+ + k_-}e^{-\left(k_+ + k_-\right)t} = \frac{1}{e^{\beta\Delta}+1} + \frac{e^{\beta\Delta}}{e^{\beta\Delta}+1}e^{-\left(k_+ + k_-\right)t}}.$$

(a) What is the "folding problem" for proteins? What is the "design problem"? Explain briefly.

The "folding problem" is the problem of, given an amino-acid sequence, finding the structure to which it folds, i.e., finding whether it has a "native state" (a unique ground state). If it does have a "native" state, then there is also the question of whether it can "find" that state starting from a random-coil configuration in a "reasonable" amount of time.

The "design problem" is the problem of, given a folded structure, finding the sequence or sequences (if any) which have that structure as the native state.

(b) Biological proteins fold due to hydrophobic repulsion. Suppose that 20% of the amino acids are hydrophobic and that an amino acid has a typical radius of 0.3 nm. Estimate the temperature at which a protein "denatures" (i.e., unfolds into the random-coil state).

For the random-coil configurations, $F_{coil} \sim -k_B T \ln z$, where z is the number of configurational choices at each link.
For the compact configurations, $F_{compact} \sim -|\varepsilon| N$, where ε is the mean hydrophobic energy benefit of hiding the hydrophobic residues.
We expect denaturation when the two are equal, i.e., when $k_B T_{denature} = \frac{|\varepsilon|}{\ln z}$.
To estimate thee quantities, assume that the hydrophobic energy of one amino acid can be calculated as $\sigma A = 4\pi\sigma R^2$ (this is an overestimate, since the residue is protected from water on the surfaces along the backbone). Thus, we estimate $k_B T_{denature} = \frac{0.2\left(4\pi R^2\right)\sigma}{\ln z} \sim \frac{0.2\left(4\pi\left(3\times 10^{-10}\right)^2\right)0.04}{\ln 6}$.
This leads to an estimate of $T_{denature} \sim 366\,K$.
This is very crude but it is at least the right order of magnitude.